

Transport properties and asymmetric scattering in $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ single crystals compared to the electron doped counterparts $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$

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Resistivity, Hall effect and magnetoresistance have been investigated systematically on single crystals of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ranging from undoped to optimally doped regions. A systematic evolution of the quasiparticle scattering has been observed. It is found that the resistivity in the normal state of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ is insensitive to the potassium doping concentration, which is very different from the electron doped counterpart $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$, where the resistivity at 300 K reduces to half value of the undoped one when the system is optimally doped. In stark contrast, the Hall coefficient R_H changes suddenly from a negative value in the undoped sample to a positive one with slight K-doping, and it keeps lowering with further doping. We interpret this dichotomy due to the asymmetric scattering rate in the hole and the electron pockets with much higher mobility of the latter. The magnetoresistivity shows also a non-monotonic doping dependence indicating an anomalous feature at about 80 K to 100 K, even in the optimally doped sample, which is associated with a possible pseudogap feature. In the low temperature region, it seems that the resistivity has the similar values when superconductivity sets in disregarding the different T_c values, which indicates a novel mechanism of the superconductivity. A linear feature of resistivity ρ_{ab} vs. T was observed just above T_c for the optimally doped sample, suggesting a quantum criticality.

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I. INTRODUCTION

The discovery of iron-based superconductors [1] has triggered great interests in the field of condensed matter physics. A lot of theoretical and experimental works suggest complicated Fermi surfaces and unconventional pairing mechanism[2–8]. There is a common issue between the iron pnictides and the cuprates, that in both systems the superconductivity is in the vicinity of the antiferromagnetic (AF) order, leading to a very similar phase diagram. However, the feature of the undoped parent phase is actually quite different. The cuprate may be categorized as the so-called Mott insulator, while the iron pnictide is a poor metal. The phase diagram has thus been a focus of intense research in order to pursue an understanding of the relationship between the AFM and the superconducting (SC) states, and intimately the superconducting mechanism[9–13]. For the electron doped 122 family, such as $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$, a lot of works both in experiment and theory illustrate the systemic evolution of the transport properties and electronic structure, all indicate the importance of the multiband effect[10, 14–18]. It was presumably believed that in the underdoped regime, the AF and the SC phase compete for the density of states along the Fermi surfaces. In the overdoped regime superconductivity suffers from a suppression of the spin fluctuations[15], and probably the loss of the Fermi surface nesting. These two effects lead to an asymmetric superconducting dome, which is somewhat different from the case in the cuprate superconductors. By analyzing the transport [10] and optical data[16, 19] in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$, it has been consistently claimed that

the mobility of the electron band are much higher than that in the hole band. It is curious to know in a hole-doped sample, would the mobility disparity survive, disappear, or change sign? In this paper we report the systematic studies on resistivity, Hall effect and magnetoresistivity on selected hole doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ single crystals. The detailed investigations and analysis suggest the asymmetric quasiparticle scattering in the hole and electron band, with still a much larger mobility in the electron band. Meanwhile we present the evidence that the electron doping induced by substituting the Fe sites with Co results in a great impurity scattering, but without breaking too much Cooper pairs. These Fe-sites doping may generate the impurities which can only scatter the electrons with small momentum transfer, with the inter-pocket pairing un-intact.

II. EXPERIMENTAL

The $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ single crystals were grown by self-flux method using FeAs as the flux, detailed procedures of synthesizing the samples are similar to the previous reports[21–23]. The crystal structure and chemical composition were checked by X-ray diffraction and energy dispersive X-ray microanalysis. For the transport measurements, all the samples were cut into rectangular shape and the standard six electric probes were made by silver paste. The electronic transport measurements were carried out in a Physical Properties Measurement System (PPMS, Quantum Design) with the temperature down to 2 K and magnetic field up to 9 T. The superconducting

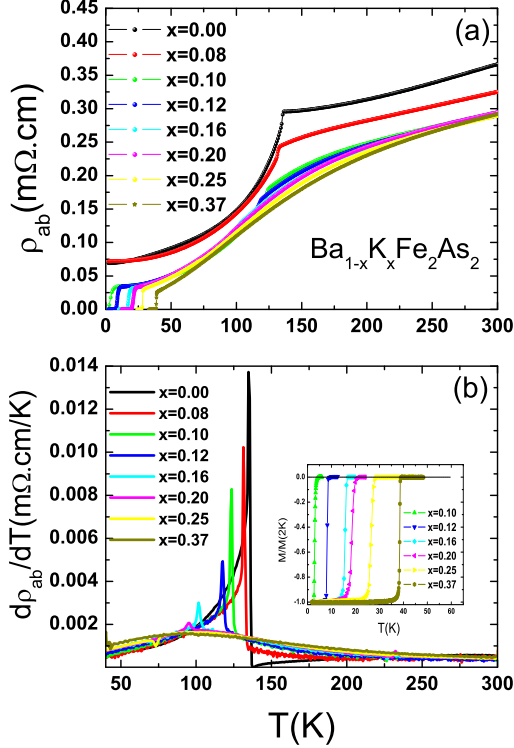


FIG. 1: (Color online) (a) Temperature dependence of resistivity of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ($x=0 \sim 0.39$) single crystals. The AF / structural transition is shifted to lower temperatures and becomes invisible with further potassium doping. The resistivity anomaly in normal state can not be explicitly resolved when the doping level is 0.25 with $T_c = 29$ K, and beyond. (b) Temperature dependence of derivative of the resistivity $d\rho_{ab}/dT$. The peak in $d\rho_{ab}/dT$ associated with the AF / structural transition is suppressed with doping and disappears at $x = 0.25$. Inset: Zero field cooling magnetization of six superconductive samples.

transition temperature of the samples were determined by the 50% of the normal state resistivity. The in-plane longitudinal and the Hall resistance were measured by either sweeping the magnetic field at a fixed temperature or sweeping the temperature at a fixed magnetic field. Both sets of data coincide with each other.

III. RESULTS AND DISCUSSION

A. Temperature and doping dependence of resistivity

Fig.1(a) shows the temperature dependence of resistivity for $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ single crystals with doping levels ranging from undoped parent phase to optimally doped compounds. It is clear that the potassium doping makes the system evolve from AF (with a resistivity anomaly) to

superconductive. The sharp drop of resistivity at about 138 K due to the AF / structural transition can be observed in the parent phase. With doping holes, the resistivity anomaly is suppressed and shifts to lower temperatures, which is agreeable with the peak in the derivative of the resistivity $d\rho/dT$ shown in Fig.1(b). When the doping level x reaches 0.25, the resistivity anomaly disappears and a little pit can be observed in $d\rho/dT$ where the superconducting transition temperature is 29 K. With further doping, the T_c reaches a maximum value at 39 K. For the electron-doped Fe-based 122 family, the magnetic and structural transition are slightly separated[21] leading to two close peaks on the $d\rho/dT$ vs. T curves. The resistivity anomaly exhibits two kinks which are corresponding to the two peaks in $d\rho/dT$ for the underdoped samples. While for hole-doped BaFe_2As_2 , some experiments show that the AF and structure transition occur at the same temperature in underdoped region [12, 13, 24]. In our measurements, we observed only one single sharp peak in $d\rho/dT$ vs. T curves for underdoped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ which is agreeable with previous results.

Here we would like to emphasize several contrasting issues by comparing the resistivity curves in electron doped $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ (Co-122)[10] and hole doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ (K-122) samples (Fig.1). Firstly, in the Co-122 samples, the resistivity at 300 K reduces to half value of undoped sample when the system is optimally doped [10], this is actually not the case in the K-122. One can see from Fig.1(a) that, the resistivity at 300 K drops only about 20-30% when the doping is getting to the maximum value. What is more interesting is that the resistivity value when the superconductivity sets in is quite close to each other although the T_c changes from 10 K ($x=0.10$) to 29 K ($x=0.25$). This may suggest the resistivity is mainly dominated by the electron band, which is weakly influenced by the hole doping. The interest triggered by this observation is two fold: the threshold for the occurrence of the superconductivity is governed by the residual resistivity at T_c , while the T_c value is determined by the hole concentration, perhaps by how strong the suppression to the antiferromagnetic phase is. It is not clear at this moment what leads to this strange behavior, but clearly it indicates a novel mechanism of the superconductivity. Secondly, the resistivity exhibits an up-rising step at the AF/structural transition in the electron doped Co-122, while in K-122, this transition exhibits always as a drop of resistivity at T_{AF} and it is smeared up gradually with more doping. Thirdly, the RRR, namely the ratio between the room temperature resistivity and the residual resistivity (just above T_c) is about 2.4 in Co-122,[10] indicating a strong impurity scattering. But it seems such a strong scattering does not block the superconductivity. Based on the picture of pairing through inter-pocket scattering,[2, 3] the non-magnetic impurities may be detrimental to the superconductivity if they induce the inter-pocket scattering. In this sense, the impurities here may induce the scattering only with small momentum transfer, for example,

intra-pocket scattering. In the optimally hole doped samples, the RRR can get to 14, indicating a weak impurity scattering. At high temperatures, the ρ_{ab} -T curve shows a bending down feature for the hole doped samples. In the conventional single band metal, the bending down of resistivity was interpreted as the approaching to the Ioffe-Regel limit, which is corresponding to the case that the mean free path induced by the phonon scattering is comparable to the atomic lattice constant. This seems not the case here, since the electron doped sample Co-122 has the same structure and similar phonon spectrum, but the bending down feature of resistivity has not been observed up to 300 K.

Above mentioned behavior of the resistivity can be qualitatively understood by the two band scenario with asymmetric scattering rate in the hole and the electron pockets. According to the simple two band model, the conductivity can be written as $\sigma = \sum_i \sigma_i$, with $\sigma_i = n_i e^2 \tau_i / m_i$ the conductivity, n_i the charge carrier density, τ_i the relaxation time, m_i the mass of the i -th band ($i = e$ or h for the electron and hole band, respectively). Therefore the resistivity can be described as

$$\rho = \frac{m_e m_h}{e^2 (n_e \tau_e m_h + n_h \tau_h m_e)}. \quad (1)$$

It is known that the parent phase has identical area of electron and hole Fermi surfaces in the non-magnetic phase, therefore we can assume an identical charge carrier densities n_e and n_h for the two bands ($n_e \approx n_h \approx n_0$). Considering $m_h > m_e$ as revealed by ARPES[25] and specific heat[26], and assuming that $\tau_e > \tau_h$, the conductivity is thus dominated by electron band. With the electron doping, the term $n_e \tau_e m_h$ is getting much larger than $n_h \tau_h m_e$ which reduces the resistivity further. To the optimally doping at about $x = 0.08$, n_e has increased a lot, perhaps doubled, this reduces the resistivity to almost its half. In the case of K-122, the situation is different. If still adopting the relation of $n_e \tau_e m_h \gg n_h \tau_h m_e$, doping holes will decrease n_e but increase n_h , in this case the resistivity should increase, instead of decrease. Actually doping holes will on one hand decrease n_e and increase n_h , but more important is to lower down the m_h and $1/\tau_h$, in this case, the resistivity will be determined by a balance between these quantities and shows a weak doping dependence. A quantitative understanding would require a detailed doping dependence of n_i , τ_i , m_i ($i = e, h$). This is out of the scheme of what we can get from a simple resistivity measurement and analysis. Some calculations indicate that the conductivity for electrons grows strongly upon electron doping, while the hole conductivity varies weakly compared to that of the electrons[27]. Thus the resistivity of hole-doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ at 300 K changes less than that for electron-doped $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$. The multi-band effect that one band is strongly coupled and relatively clean, while the other band is weakly coupled and characterized by much stronger impurity scattering will cause

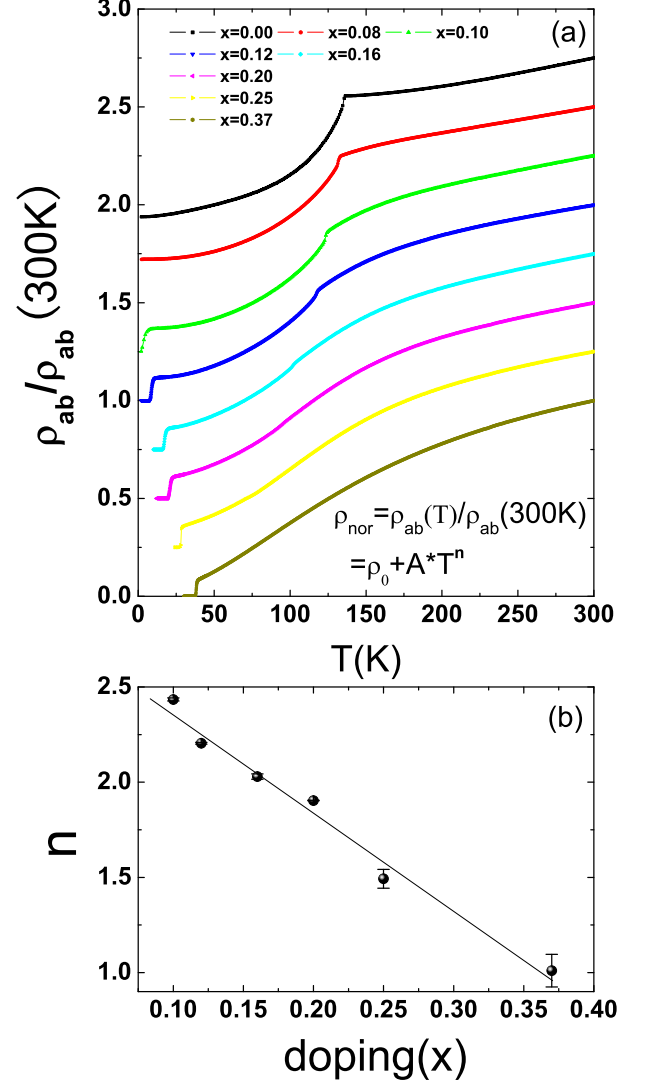


FIG. 2: (Color online) (a) Temperature dependence of the normalized in-plane resistivity ($\rho_{ab}/\rho_{ab}(300\text{K})$) of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$. The data sets are offset vertically by 0.25 for clarity. (b) The fitting parameter n for six doped superconducting samples (see text).

anomalous T-dependence of the in-plane resistivity: the curve is convex with the tendency to saturate at high temperature[28].

B. Trace of possible quantum critical point at the optimal doping

In Fig.2(a) we present temperature dependence of the normalized ρ by the room temperature resistivity $\rho_{ab}(300\text{K})$. A quick glance at the data can immediately see that the ρ -T curve in the low temperature region

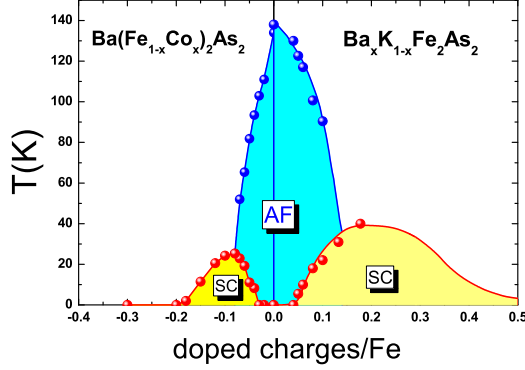


FIG. 3: (Color online) The phase diagram of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$. No splitting between the structural and AFM transitions has been observed in the hole doped samples. The curve of T_c vs. doping in wide hole doping region (solid line) was taken from the Ref.[12]. The data in the electron doped regions were adopted from Ref.[10].

changes from a non-linear to a linear behavior towards optimal doping. In order to know precisely the evolution of the resistivity with doping, we fit the data in the low temperature region by the equation

$$\rho_{\text{nor}} = \rho(T)/\rho(300\text{K}) = \rho_0 + A \times T^n \quad (2)$$

with three fitting parameters ρ_0 , A and n for each curve. Due to the saturation in the resistivity at high temperatures and the anomalies of resistivity induced by the AF/structure transition, we fit the data below the AF/structure transition (for $x=0.25$ and below). For the optimally doped sample, the fitting was done with the data between 40 and 120 K. The resulted fitting parameters are presented in Table I and the exponent n is shown in Fig.2(b). The evolving from a power law with exponent $n = 2.3$ to a linear temperature dependence can be easily observed in Fig.2(b), which may indicate the crossover from a Fermi liquid behavior to non-Fermi liquid when the quantum critical point is approached. It was previously pointed out that the exponent n in metals near an AFM quantum critical point (QCP) may be sensitive to disorder[29]. While in K-122 the impurity scattering is quite weak, this can be corroborated by the negligible ρ_0 value at the optimal doping. At the optimal doping, the T-linear resistivity in the low temperature region may suggest a quantum critical point. Similar behaviors have been observed in $\text{Sr}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ [30], $\text{BaFe}_2\text{As}_{2-x}\text{P}_x$ [31], $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ [15] etc.. It has been pointed out that the quantum fluctuation becomes very strong when the Neel temperature of the AFM order becomes zero. It is this strong quantum fluctuation that heavily couple to the itinerant electrons and modifies the transport property. Although it was argued that this linear feature may be reconstructed with a residual term and a T^2 term in the optimally doped

$\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ system,[20], the systematic evolution shown in our present study can rule out this possibility.

For the cuprate superconductors, the antiferromagnetic order of the magnetic moments of the Cu^{2+} is completely suppressed before superconductivity sets in. They do not coexist at any point of the $T_c(p)$ (p : doped hole number) phase diagram (exception was suggested in the Bi-2201 system). In contrast, the coexistence of the AFM and the superconductivity can be observed in underdoped region of the dome of K-122 [13, 15, 24, 32, 33]. Fig.3 shows the phase diagram of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$. Although there are some reports claiming that magnetically ordered phases and SC state are probably mesoscopically/microscopically separated [36–38], most of the studies on K or Co doped samples are in favor for the coexistence of magnetic order and superconductivity and have consistently ruled out the presence of phase separation[15, 33, 34]. The very small residual specific coefficient γ_0 in the optimally doped $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ also strongly suggest the absence of macroscopic phase separation, since otherwise one should be able to see a large residual term of specific heat. Therefore we argue that the QCP occurs near the optimally doped samples where the AFM order vanishes at about zero K. In the specific heat measurements, we also found that the mass enhancement m^*/m goes up quickly when the optimally doping point is approached.[35] To confirm the existence of quantum critical point and the coexistence of magnetic order and superconductivity need certainly extra investigations using other local probes.

TABLE I: Fit Parameters

x	ρ_0	A (10^{-5})	n
0.10	0.117 ± 0.00038	0.54 ± 0.0139	2.33 ± 0.00324
0.12	0.114 ± 0.00025	1 ± 0.026	2.20 ± 0.00482
0.15	0.096 ± 0.00102	3 ± 0.187	2.02 ± 0.0139
0.20	0.091 ± 0.00007	5 ± 0.037	1.90 ± 0.0017
0.25	0.057 ± 0.00263	32 ± 7	1.49 ± 0.04921
0.39	-0.005 ± 0.00349	359 ± 57	1.01 ± 0.1566

C. Temperature and doping dependence of Hall coefficient

The Hall coefficient R_H from undoped BaFe_2As_2 to optimally doped K-122 are presented in Fig.4(a) and the systematic evolution can be observed. The Hall coefficient R_H changes suddenly from a negative value in the undoped sample to a positive one with slight K-doping, and it keeps lowering with further doping in low temperature region. For each doping level, the sudden increase of the Hall coefficient is corresponding to the AF/structure transition which is agreeable with the resistivity anomaly for underdoped K-122 ($x = 0.1 \sim 0.25$).

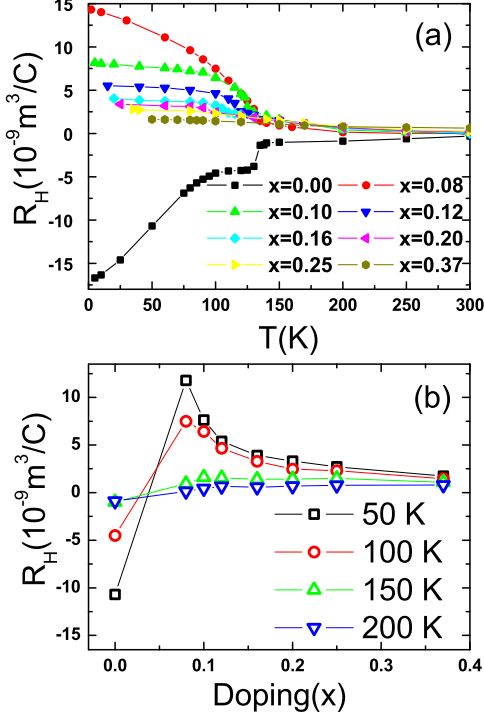


FIG. 4: (Color online) (a) The temperature dependence of Hall coefficient of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ($x = 0 \sim 0.37$). The Hall coefficient R_H changes suddenly from a negative value in the undoped sample to a positive one with slight K-doping. The AF/structure transition can be found in the underdoping dome ($0.08 \leq x \leq 0.25$) as an onset of the rising of the Hall coefficient R_H . For the optimal doped sample, R_H varies less pronounced with the temperature. (b) The doping dependence of Hall coefficient at different temperatures.

Above the AF/structure transition temperature the Hall coefficient varies weakly. The general formula for the Hall coefficient in the Boltzmann approximation reads

$$R_H = \sum \frac{\sigma_i^2}{en_i} / (\sum \sigma_i)^2 \quad (3)$$

For fully compensated semimetals within the two-band model, Eq.3 reduces to

$$R_H = \frac{n_h \mu_h^2 - n_e \mu_e^2}{e(n_e \mu_e + n_h \mu_h)^2}. \quad (4)$$

By definition, undoped samples are compensated, that is, $n_h = n_e = n_0$. The Eq. 4 can be written as

$$R_H = n_0^{-1} \frac{\mu_h - \mu_e}{\mu_h + \mu_e} = n_0^{-1} \frac{\sigma_h - \sigma_e}{\sigma_h + \sigma_e}, \quad (5)$$

where $\mu_i = \sigma_i/n_i = \tau_i/m_i$ ($i = e, h$) is the mobility. If $\mu_e \gg \mu_h$, then $R_H \approx 1/en_e$, the transport is dominated by the electron band[10]. However, with the potassium doping, the hole pocket increases in size instantly

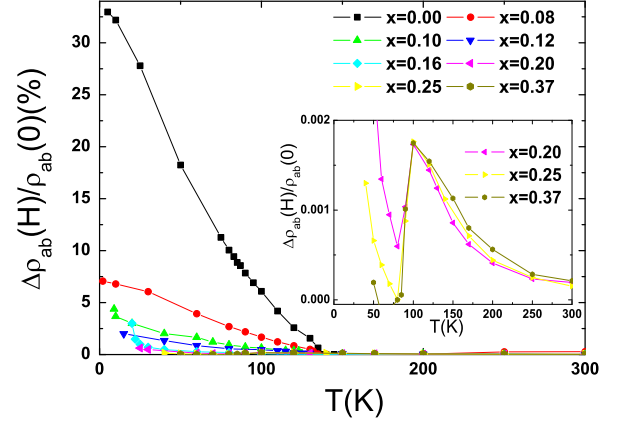


FIG. 5: (Color online) Temperature dependence of magnetoresistivity for $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ($x=0 \sim 0.37$) measured at 9 T. Inset: magnetoresistivity of the samples ($x=0.2, 0.25, 0.37$). An anomaly at around 80-100 K can be easily observed.

and the electron pocket contracts. At the hole doping with an $x \sim n_0$, the Hall coefficient changes sign. With further doping, the hole-doped systems have a presence of γ pocket near (π, π) . In addition to $(\pi, 0)$ scattering between α and β sheets, new phase space for scattering opens up.[27]. The asymmetric scattering rate in the hole and the electron pockets play an important role on R_H . Fig.4 shows the doping dependence of Hall coefficient at 50 K, 100 K, 150 K, 200 K. In low temperature region, R_H changes sign and reaches a large value with little potassium doping. With further doping, R_H decreases gradually. In high temperature region the R_H varies very little, which is agreeable with the recent calculation[27]. In the electron doped 122 system, the transport property is dominated by electron. In compensated case, the results can be explained by remarkable different mobilities of hole and electrons[10]. For hole doped K-122, the asymmetric scattering rate in the hole and the electron pockets still holds, but the relative ratio between τ_e/m_e and τ_h/m_h may change a little bit, namely τ_h/m_h will get enhanced. This is especially necessary to interpret the dropping down of resistance at high temperatures when the slight holes are doped into the system, as shown in Fig.1.

D. Magnetoresistance

The temperature dependence of magnetoresistivity for nine samples measured at a magnetic field of 9 T are presented in Fig.5. The data shows also a non-monotonic doping dependence and a sudden increase below AF/structure transition, which is associated very well with the anomaly found in resistivity and Hall effect.

In undoped sample, the large magnetoresistivity with a magnitude of about 35% (at about 9 T) has been found in low temperature region. With increasing doping, the magnetoresistivity decreases instantly. It remains unclear yet what causes this large magnetoresistance within the AF phase. There are two main explanations: (1) The magnetic field will break down the antiferromagnetic order to some extent and lead to stronger spin fluctuations and thus larger scattering to itinerant electrons; (2) A magnetic field will induce a stronger localization leading to an enhanced resistivity.

In addition to this strong magnetoresistance in the antiferromagnetic state, an anomalous feature at about 80 to 100 K can be observed even in the optimally doped sample in which the AF state does not exist at all. One can see this in the inset of Fig.5. The magnetoresistance rises up gradually when the temperature is lowered down, but it drops suddenly at about 100 K and reaches almost zero (for the optimally doped sample), then it rises up again in the lower temperature region and smoothly connected to the magnetoresistance induced by the vortex motion in the mixed state. This anomaly at about 100 K may be associated with a possible pseudogap feature due to some unknown reasons. This is consistent with the recent observation in the c-axis resistive measurements where a maximum of ρ_c is observed.[18] A high temperature pseudogap was also claimed very recently from the optical conductivity measurements.[40] Further experimental and theoretical investigations are needed to clarify this point.

IV. CONCLUSIONS

In summary, we investigated resistivity, Hall effect and magnetoresistance systematically on single crystals of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ranging from undoped to optimally doped samples. The resistivity in the normal state of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ is insensitive to the potassium doping compared to the electron doped $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ samples. The Hall coefficient R_H changes suddenly from a negative value in the undoped sample to a positive one with slight K-doping, and it keeps lowering with further doping. This contrasting behavior is interpreted as due to the asymmetric scattering between the electron and hole bands with the much larger mobility in the former. An anomalous feature of magnetoresistivity has been observed at about 80 to 100 K and may be associated with a possible pseudogap feature. A linear feature of resistivity ρ vs. T was observed just above T_c for the optimally doped sample, which suggests a quantum criticality.

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